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Full Paper

Volatile profiles of tomato wine before and after ageing

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Abstract: The volatile profiles of tomato wine before and 90 days after storage at 10° and 15° were determined. The results indicate that storage temperature significantly influences the volatile composition of tomato wine. A total of 75 volatile compounds are identified, viz. 38 esters, 7 carbonyls, 1 furan, 4 sulphur-containing compounds, 18 higher alcohols, 6 fatty acids and 1 terpene. Twenty-five volatile compounds are present beyond their odour threshold, but the major contributors to the overall aroma of tomato wine are ethyl octanoate, ethyl hexanoate and isoamyl acetate, which are characterised by fruity notes. The potent odoriferous volatile compound, linalool, contributes much to the wine stored at 15° than at 10°. Storage significantly improves the fruitiness of tomato wine.

Keywords: tomato wine, volatile profile, aroma, odour threshold, wine ageing

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INTRODUCTION

The aroma of wine influences its quality, cost and consumer choice. A mix of numerous and unique odour compounds contributes to the complexity of wine aroma [1]. Over 800 volatile compounds have been identified in wines [2]. The volatile composition of wine is influenced by several factors including the type and variety of fruit [3], yeast strain [4], inoculum size [5], fermentation temperature [6], maturation process and type of ageing [7]. In order to produce wine of the best flavour, the concentration of desirable volatile compounds should be enhanced and that of undesirable ones minimised [8]. During fermentation, the growth and development of yeast and the formation of flavour compounds are influenced by many factors such as yeast strain, pH, temperature and inoculum size.

Tomato is one of the most important vegetables in the world, with the total production of 145.8 million tonnes recorded in 2010 and 161.79 million tonnes in 2012 [9]. Fruits and vegetables including tomato are reported to experience post harvest losses of about 20-50%, especially in the developing world. Many fruits have been utilised for winemaking [3, 4] as a means of stemming postharvest losses, and tomato can also be considered a potential candidate with its unique phytochemical and flavour composition [10, 11]. The unique flavour is due to a complex mixture of volatile and non-volatile compounds: over 400 volatile compounds have been identified in tomato [12, 13]. However, compounds that appear to be the most important determining factors of flavour in tomato are *cis*-3-hexenal, hexenal, 2-isobutylthiazole, β-ionone, *trans*-2-hexenal, *cis*-3-hexenol, *trans*-2-*trans*-4-decadienal, 6-methyl-5-hepten-2-one and 1-penten-3-one [13]. The aroma of fresh tomato is quite different from that of the processed one as a result of loss and creation of volatiles [14]. Increased concentration of linalool and α-terpineol was reported for heated tomato [12]. Likewise, winemaking, which involves maceration, fermentation, maturation and ageing, is likely to modify the volatile composition of tomato wine. This modification should be controlled in order to produce tomato wine of acceptable aroma. Among the many factors which can be controlled to modify tomato wine aroma are pH of the must, fermentation and ageing temperature.

Many authors have studied the volatile composition of many fruits and their wines [3-5, 15-18]. However, to the best of our knowledge, even though the volatile profile of tomato has been studied extensively [e.g. 19, 20], that of its wine has not been reported before. The aim of this study is therefore to assess the volatile profile of tomato wine before and after storage in order to evaluate how it influences tomato wine quality.

MATERIALS AND METHODS

Preparation of Yeast Culture

The dry yeast used, *Saccharomyces bayanus*, BV 818, was purchased from Angel Yeast Company Limited, Hubei province (China) and kept in a refrigerator at 5^{o}C according to the manufacturer's instructions. The yeast culture was prepared in YDP medium (yeast extract = 0.5% (w/v), peptone = 1.0% (w/v) and glucose = 2% (w/v)) in a 250-mL Erlenmeyer flask. The pH of the culture medium was adjusted to 5.0 with tartaric acid. The medium was sterilised in an autoclave at 121^{o} for 20 min. *S. bayanus*, BV 818 (0.03 g) was suspended in 100 mL of sterilised medium and heated to 40^{o} for 20 min. to rehydrate the yeast cells [21]. It was then cooled to room temperature (25^{o}) for adaptation [22] and incubated in an incubator shaker (QYC 211, Shanghai Test Equipment Co. Ltd) at 30^{o} for 24 hr.

Tomato Wine Production

Tomatoes (*L. esculentum* Mill.), was purchased from a market in Zhenjiang, Jiangsu province, were selected based on colour and size uniformity. They were washed several times with running tap water to remove dirt, sterilised with 2% potassium metabisulphite, rinsed several times with distilled water, dried with napkin paper and blended with a sterilised blender. Potassium metabisulphite (0.050 g/L) was added to the must as an antioxidant and antimicrobial agent [22].

Pectic enzyme (0.5 g/L) (Sinopharm Chemical Reagent Co., Ltd (Shanghai)) was added to break down pectin to improve aroma and colour extraction [23], and ammonium phosphate (0.5 g/L) was added as a source of ammonia and phosphorus for the growth of the yeast [24]. The total soluble solid (TSS) of the milled tomato was measured with Abbe refractometer (WAY-2S, China) in accordance with a known method [25] and the value obtained was 4.90 ± 0.20^o Brix. The TSS of the original tomato must was ameliorated with sucrose to 20.6 ± 0.30^oBrix [26]. The pH of the must at 25^o was determined with a pH meter (PHS-2C Precision pH/mV meter, China) after standardisation with standard buffer solutions of pH 7 and 4, according to an established method [27]. The must pH obtained was 4.11. Into a 5-L Erlenmeyer flask was placed 4.5 L (5.30 kg) of tomato must, which was inoculated with 180 mL ($1.3x10^6$ cells/mL) of the 24-hr *S. bayanus*, BV 818 inoculum to give an inoculum level of 3.8%. The must was batch-fermented in triplicate in an incubator at $15{\pm}2^o$ [22]. The fermentation was monitored until the TSS value of the must became stable. After fermentation, the wine was separated from the pomace and stored at 7^o for two months for particles to settle down. The wine titratable acidity was measured as described previously [28] and the ethanol content was determined by a known method [29].

Ageing of Tomato Wine

The tomato wine samples were aged in bottles in triplicate. They were put in 250-mL brown bottles, potassium metabisulphite (0.027 g/L) was added, and the bottles were tightly capped. They were incubated at 10^o and 15^o for 90 days. Samples were taken for analysis on day 0 and 90. Analysis was done in triplicate.

Analysis of Volatile Compounds

A modified method of solid phase microextraction (SPME) technique described by Márquez et al. [30] was used for extraction of volatile compounds from tomato wine. The SPME fibre used was a Stable Flex divinylbenzene/Carboxen/polydimethylsiloxane (DVB/CAR/PDMS) (Supelco, Bellefonte, USA), which is designed for flavour analysis. The fibre was conditioned for 1 hr at 270^o before use. For each SPME analysis, 5 mL of the wine sample was placed in a 15-mL glass vial containing a small stirring magnet at 350 rpm. The sample was spiked with 50 µL of an internal standard (aqueous solution of 1-propanol (100μg/L)). Sodium chloride (1 g) was then added to increase the volatility of the flavour compounds. The vial was then sealed with a silicone septum and put into a water-bath (40^o). An SPME needle was then pierced through the septum and the SPME fibre was extended through the needle to place the stationary phase in contact with the headspace of the sample. The fibre was withdrawn into the needle after 30 min. and removed from the vial and inserted for 3 min. in the injection port of a gas chromatograph (6890/5973 GC-MS, Agilent, USA). The extracted chemicals were desorbed thermally at 250^o and transferred directly to a DB-1701 cross-linked (14% cyanopropylphenylmethylpolysiloxane) column (30 m, 0.25 mm i.d., 25-µm film thickness) (Agilent, USA).

The injection port was operated in splitless mode and the flow rate of helium (99.9995%) as carrier gas was 1 mL/min. The initial oven temperature was held at 50^o for 10 min., ramped at 6^o/min to 150^o, and then at 8^o/min to 200^o and held for 3 min. The total run time was 35.9 min. The Agilent 5973 quadrupole mass spectrometer was operated in the electron ionisation mode at 70 eV with a source temperature of 230^o (quadrupole at 150^o), with a continuous scan from *m*/*z* 33 to *m*/*z* 330. The data were collected with HP ChemStation software (D.00.00) and searched against the NIST98 libraries. Compounds were preliminarily identified by a library search and their identities

Maejo Int. J. Sci. Technol. **2014**, *8*(02), 129-142

were confirmed by mass spectra and GC retention time of standards or a homologous series of straight chain alkanes (C5-C19). The quantitation of the volatile compounds was based on peak surface areas in the chromatograms. All tests were carried out in triplicate.

Determination of Odour Activity Values

The odour activity values (OAVs) were determined as the ratio of the mean concentration of an aroma compound to its odour threshold value (the lowest concentration that can be detected through smell) obtained from the literature. The aroma compounds with OAVs greater than 1 were considered as those which contribute to the aroma of the wine [31].

Data Analysis

All data were expressed as mean ± standard deviation and subjected to Analysis of Variance (ANOVA) using SPSS Version 17.0. The differences in means were separated with Duncan's Multiple Range test and $P<0.05$ indicated that the difference was significant.

RESULTS AND DISCUSSION

General Attributes

After ageing the pH and titratable acidity of the tomato wine decrease slightly but are not significantly different ($P>0.05$) from those before (Table 1). The pH values are comparable to those regarded suitable for white and red wines [22]. In addition, the TSS and ethanol content of the wine after ageing are similar to those before ageing.

Table 1. General wine attributes before and after ageing

Attribute	pH	TA (g/L)	TSS (^{o}Brix)	EC (g/L)
C	3.67 ± 0.01^{a}	4.43 ± 0.33^{a}	6.0 ± 0.3^{a}	71.10 ± 6.32^{a}
C10	3.60 ± 0.00^{a}	4.40 ± 0.40^{a}	6.50 ± 0.30^{b}	67.15 ± 3.16^{a}
C15	3.60 ± 0.00^{a}	4.40 ± 0.40^{a}	6.20 ± 0.30^{a}	68.73 ± 3.95^{a}

Note: C = tomato wine before ageing; C10 = tomato wine after ageing at 10^{o}; C15 = tomato wine after ageing at 15^{o}; TA = titratable acidity; TSS = total soluble solid; EC = ethanol content. Means with the same alphabets in a column are not significant at $P<0.05$. Mean ± standard deviation were obtained from triplicate measurements.

Volatile Compounds

The total number of volatile compounds identified in tomato wine before and after storage are 75 (Table 2). These comprise 38 esters, 7 carbonyls, 1 furan, 4 sulphur compounds, 18 higher alcohols, 6 fatty acids and 1 terpene. Most of the volatiles identified are known compounds in wines and are mainly formed during the fermentation and winemaking processes [32].

Maejo Int. J. Sci. Technol. **2014**, *8*(02), 129-142

Table 2. Concentrations of volatile compounds (mg/L) in fresh tomato wine and those aged at 10° and 15°

Compound	C	C10	C15	Odour threshold	Odour descriptor
Esters					
Ethyl acetate	14.13 ^{a} ±0.03	15.86 ^{b} ±0.04	16.89 ^{c}±0.06	7.5	Fruity, sweet
Ethyl propanoate	-	0.18^{b} ±0.00	0.22^{c}±0.01	0.01	Fruity
Ethyl butanoate (Ethyl butyrate)	2.71^{a} ±0.02	2.98^{b} ±0.03	3.55^{c} ±0.04	0.02	Floral, fruity
Ethyl pentanoate	0.45^{c} ± 0.00	0.26^{b} ±0.01	0.12^{a} ±0.00	-	-
Ethyl hexanoate	71.54^{a}± 0.43	81.09^{b} ±0.27	104.34^{c}±0.43	0.014	Apple, fruity, sweetish
(Z)-Ethyl-3-hexenoate	0.33^{a} ±0.01	0.40^{b} ±0.02	0.51^{c} ±0.02	-	-
Ethyl heptanoate	1.08^{a} ±0.03	1.67^{b} ±0.03	1.87^{c} ±0.04	-	Wine-like, fruity
Ethyl-6heptenoate	0.16 ±0.01	ND	ND	-	-
Ethyl octanoate (EO)	346.63^{a} ±1.13	367.90^{b} ±0.97	366.63^{b} ±1.21	0.02	Sweet, fruity and fresh
% EO of all esters	68.19	59.08	59.44	-	-
(Z)-Ethyl-3-octenoate	ND	ND	0.49 ±0.02	-	-
Ethyl nonanoate	ND	1.14^{a} ±0.03	0.70^{a} ±0.01	0.38	Cognac, fatty, oily
Ethyl-8-nonenoate	ND	0.50 ±0.03	-	-	
Ethyl decanoate	30.44^{a} ±1.01	100.09^{c} ±1.04	75.39^{b} ±0.43	1.5	Flowery, fruity
Ethyl-9-decenoate	5.50 ^{a} ±0.06	16.66 ^{c} ±0.08	12.50 ^{b} ±0.05	-	Fatty, fruity
Ethylbenzoate	ND	0.37^{a} ±0.02	0.41^{b} ±0.01	-	Floral, fruity
Ethyl-3-cyclo-pentyl propionoate	0.63 ±0.03	ND	ND	-	-
Diethyl ethanoate	0.26 ±0.01	ND	ND	-	-
Diethyl succinate	1.73^{a} ±0.03	2.82^{c} ±0.02	2.21^{b} ±0.01	0.07	Light fruity
Methyl acetate	ND	0.11 ±0.01	ND	-	Ethereal, estery, fruity
Isoamyl acetate	17.32^{b} ±0.02	15.76^{a} ±0.05	18.58^{c} ±0.02	0.03	Banana, pear
Ethyl 3-methyl butanoate	0.93^{c} ±0.01	ND	ND	-	Fruity
Isoamyl octanoate	2.44^{b}±0.02	3.87^{c}±0.03	2.23^{a} ±0.04	-	-
Methyl hexanoate	-	0.24^{a} ±0.02	0.32^{c} ±0.01	-	-
Methyl octanoate	6.13^{b} ±0.03	5.66^{a} ±0.12	6.13^{b} ±0.13	0.20	Intense citrus
Methyl decanoate	ND	1.17 ±0.03	ND	-	Fatty, cognac, oily
Propyl hexanoate	0.13^{a} ±0.01	0.28^{b} ±0.02	0.37^{c} ±0.00	-	-
Propyl octanoate	ND	ND	0.83 ±0.02	-	Coconut, fatty, winey
Butyl butanoate	0.46 ±0.02	ND	ND	-	-
Isobutyl pentanoate	ND	0.30 ±0.00	-	-	-
Isobutyl octanoate	ND	0.28^{b} ±0.00	0.17^{a} ±0.00	-	Fatty, fruity, winey
2-Butyl octanoate	0.11 ±0.00	ND	ND	-	-
Isopentyl hexanoate	ND	ND	1.86^{c} ±0.12	-	-
Hexyl acetate	0.24^{a} ±0.00	0.46^{b} ±0.01	0.45^{b} ±0.01	0.7	Sweet, perfume
Hexyl octanoate	0.61^{a} ±0.03	ND	ND	-	-
2-Phenylethyl acetate	ND	2.50 ±0.02	ND	0.25	Floral, rose, fruity, honey

Note: Values are means ± standard deviation obtained from triplicate measurements. C = tomato wine before ageing; C10 and C15 = tomato wines aged at 10° and 15° respectively; ND = not detected; ' -' = no data/information. Means with the same alphabets in a row are significant (P<0.05).

Maejo Int. J. Sci. Technol. **2014**, *8*(02), 129-142

Table 2. (Continued)

Compound	C	C10	C15	Odour threshold	Odour descriptor
2-Hydroxymethyl benzoate	ND	0.18 ±0.01	ND	-	-
2-Phenylethyl 4-fluorobenzoate	4.39 ±0.04	ND	ND	-	-
Subtotal (mg/L)	**508.35^{a}±2.98**	**622.73^{c}±2.91**	**616.77^{b}±2.68**		
Subtotal (%)	**68.46**	**82.39**	**78.82**		
Carbonyls					
Acetaldehyde	0.8^{a} ±0.07	1.45^{b} ±0.05	1.36^{b} ±0.05	100	Sherry, nutty, bruised apple
Butanal	ND	ND	0.02 ±0.01	-	-
Decanal	1.28 ±1.05	ND	ND	1.0	Grassy, orange skin-like
2-Cyclohexene-1-one	ND	0.50 ±0.00	ND	-	-
6-Methyl-5-hepten-2-one	3.33^{c} ±0.07	1.61^{a} ±0.11	2.23^{b} ±0.05	-	-
% 6-Methyl-5-hepten-2-one of carbonyls	50.45	22.61	39.40	-	-
3-Octanone	0.72^{a} ±0.05	ND	ND	-	-
(E)-5,9-Undecadien-2-one	0.46^{a} ±0.02	3.56^{c} ±0.01	2.05^{b} ±0.03	-	-
Subtotal (mg/L)	**6.60^{b} ±1.26**	**7.12^{b} ±0.17**	**5.66^{a} ±0.14**	-	-
Subtotal (%)	**0.89**	**0.94**	**0.72**		
Furans					
2,3-Dihydrobenzofuran	4.23 ±0.04	ND	ND	-	-
Subtotal (mg/L)	**4.23 ±0.04**	ND	ND		
Subtotal (%)	**0.57**	ND	ND		
Sulphur compounds					
Thiazole	0.20 ±0.01	ND	ND	0.038	Popcorn, peanut
2-Isobutylthiazole	ND	0.17 ±0.03	ND	-	-
3-Methylisothiazole	0.33^{b} ±0.01	ND	0.25^{a} ±0.03	-	-
5-Methylthiazole	0.20 ±0.00	ND	ND	-	-
Subtotal (mg/L)	**0.73^{c} ±0.02**	**0.17^{a} ±0.03**	**0.25^{b} ±0.03**		
Subtotal (%)	**0.10**	**0.02**	**0.04**		
Fatty acids					
Acetic acid	2.29^{a} ±0.24	3.23^{b} ±0.15	ND	200.0	Acid, fatty
3-Methylbutanoic acid	0.93^{b} ±0.01	ND	0.66^{a} ±0.00	3.0	Cheese, rancid
Hexanoic acid	12.40^{c} ±0.12	10.80^{b} ±0.43	8.70^{a} ±0.20	3.0	Cheese, rancid, fatty, fruity
Heptanoic acid	ND	1.26^{b} ±0.05	0.38^{a} ±0.32	3.0	Fatty, dry
Octanoic acid	41.75^{c} ±0.22	4.44^{a} ±0.52	36.78^{b} ±0.22	10	Rancid, fatty acid, dairy
Acetohydroxamic acid	ND	0.28 ±0.00	ND	-	-
Subtotal (mg/L)	**57.37^{b} ±0.59**	**20.01^{a} ±0.72**	**46.52^{b} ±0.22**		
Subtotal (%)	**7.73**	**2.65**	**5.94**		
Higher Alcohols					
3-Methyl-1-butanol (isoamyl alcohol)	151.35^{c} ±1.01	88.50^{a} ±1.02	98.81^{b} ±0.01	60.0	Solvent, sweet, nail polish
% 3-Methyl-1-butanol of total alcohol	92.77	85.61	89.73		
2-Methyl-1-propanol (isobutyl alcohol)	ND	3.58 ±0.02	ND	0.55	Malty
3-Ethoxy-1-propanol	ND	0.64^{b} ±0.00	0.38^{a} ±0.00	0.1	Fruity

Note: Values are means ± standard deviation obtained from triplicate measurements. C = tomato wine before ageing; C10 and C15 = tomato wines aged at 10^{o} and 15^{o} respectively; ND = not detected; ' -' = no data/information. Means with the same alphabets in a row are significant (*P*<0.05).

Maejo Int. J. Sci. Technol. **2014**, *8*(02), 129-142

Table 2. (Continued)

Compound	C	C10	C15	Odour threshold	Odour descriptor
(S)-1,3-Butanediol	ND	0.19 ±0.00	ND	-	-
2,3-Butanediol	0.46^{a} ±0.06	ND	0.52^{a} ±0.03	150	Floral, waxy, fruity, herbal
Amyl alcohol	0.62^{b} ±0.04	0.25^{a} ±0.02	0.28^{a} ±0.02	80.0	Fruity, balsamic
4-Methyl-1-pentanol	ND	ND	0.30 ±0.00	-	-
1-hexanol	3.73^{b} ±0.08	2.15^{a} ±0.31	2.60^{a} ±0.39	8.0	Green grass
(S)-(+)-3-Methyl-1-pentanol	0.66^{b} ±0.00	0.40^{a} ±0.03	0.47^{a} ±0.10	-	Fruity, balsamic
(E)-3-Hexen-1-ol	0.82^{a} ±0.24	0.50^{a} ±0.21	0.56^{a} ±0.28	0.4	Green, floral
1-Heptanol	1.70^{a} ±0.20	2.19^{b} ±0.10	1.77^{ab} ±0.30	1.0	Grape, sweet
1-Octanol	2.32^{c} ±0.05	1.88^{a} ±0.13	2.08^{b} ±0.03	0.12	Intense citrus, roses
6-Octen-1-ol	ND	0.94 (0.08)	ND	-	-
1-Nonanol	ND	ND	0.70^{a} ±0.05	0.058	-
(E)-2-Nonen-1-ol	ND	0.30 ±0.05	ND	-	-
(Z)-3-Nonen-1-ol	1.15^{c} ±0.04	0.86^{b} ±0.03	0.90^{b} ±0.05	-	-
9-Decen-1-ol	0.34^{a} ±0.03	0.59^{b} ±0.06	0.42^{a} ±0.05	-	-
Benzyl alcohol	0.40^{a} ±0.05	0.41^{a} ±0.05	0.33^{a} ±0.10	200	Citrusy, sweet
Subtotal (mg/L)	**163.15^{c}**	**103.38^{a}**	**110.12^{b}**		
Subtotal (%)	**21.97**	**13.68**	**14.07**		
Terpene					
Linalool	2.11^{a} ±0.25	2.39^{a} ±0.14	3.23^{b} ±0.45	0.025	Fruity, citric
Subtotal (mg/L)	**2.11^{a} ±0.25**	**2.39^{a} ±0.14**	**3.23^{b} ±0.45**		
Subtotal (%)	**0.28**	**0.32**	**0.41**		

Note: Values are means ± standard deviation obtained from triplicate measurements. C = tomato wine before ageing; C10 and C15 = tomato wines aged at 10^{o} and 15^{o} respectively; ND = not detected; ' -' = no data/information. Means with the same alphabets in a row are significant (*P*<0.05).

Most esters found in wines are formed mainly through yeast fermentation [22] and are the main cause of fruitiness in wines, so they play an essential role in the aroma character of young wines [33]. In this study esters are the most abundant volatile compounds, the total concentration being 508.35 mg/L (68.46% of the total volatiles). This is greater than that reported for three varietal wines (26.30-34.20%) [15]. It also increases to 622.73 mg/L (82.39% of the total volatiles) and 616.77 mg/L (78.82% of the total volatiles) when stored at 10^{o} and 15^{o} respectively. The rise in the level of esters during ageing is apparently due to chemical esterification of alcohols and acids [34]. A previous study reported an increase in total ester concentration of white wines after 12 months [35]. The major esters found in the tomato wine are ethyl octanoate, ethyl decanoate and ethyl hexanoate (Table 2). Ethyl octanoate alone constitutes 68.19% of all the esters. The concentration of ethyl octanoate increases significantly (*P*<0.05) after storage, but storage temperature effect is not significant (*P*>0.05). Ethyl octanoate is known for its sweet, fruity and fresh notes [36]. The concentration of ethyl decanoate with flowery and fruity notes [37] is also influenced significantly (*P*<0.05) by storage temperature (Table 2). The wine stored at 10^{o} records a higher value (*P*<0.05) of ethyl decanoate than does the one stored at 15^{o}. Ethyl hexanoate imparts apple fragrance to wine [38] and after storage its concentration increases significantly. The wine stored at 15^{o} gives a higher value (*P*<0.05) of ethyl hexanoate than does the one stored at 10^{o}. The other important esters detected are isoamyl acetate, ethyl acetate, ethyl 9-decenoate, ethyl butanoate, isoamyl octanoate, diethyl butanedioate and ethyl 3-methylbutanoate. The storage temperature has a significant effect (P<0.05) on the isoamyl acetate concentration. Isoamyl acetate is characterised by a banana fragrance [31]. During ageing the tomato wine stored at both temperatures records significant increase (P<0.05) in their ethyl acetate content. The ethyl acetate concentrations before and after storage are all less than 150.00 mg/L and is likely to impart a pleasant and fruity fragrance to the wine [39]. The ethyl 9-decenoate concentration is 5.50 mg/L and this increases to 16.66 mg/L and 12.50 mg/L after storage at 10^o and 15^o respectively. Ethyl butanoate contributes floral and fruity notes to wine aroma [40]. After fermentation, the ethyl butanoate concentration is 2.71 mg/L and this increases significantly (P<0.05) after storage, with the wine stored at 15^o recording the highest.

The total concentration of carbonyls recorded for the tomato wine is 6.60 mg/L (0.89% of the total volatiles). The major carbonyl detected is 6-methyl-5-hepten-2-one (3.33 mg/L, 50.45% of total carbonyls). Its concentration is influenced by storage temperature (P<0.05) and storage leads to its diminution. It is one of the compounds that represent the fresh tomato flavour [13] and is an important product of lycopene catabolism [41]. The general reduction in its content after ageing might reduce the fresh tomato flavour of the wine. The aldehydes found in wine are mostly produced through fermentation and the processing of or extraction from oak cooperage [22]. The acetaldehyde concentration of the tomato wine is 0.81 mg/L while the sensory threshold of acetaldehyde is 100 mg/L [33]. Above this threshold acetaldehyde is usually considered as an off-odour but when it combines with other oxidised compounds, it imparts fragrance to sherries. The acetaldehyde concentration in the tomato wine is far below the threshold and it is thus not expected to contribute negatively to the flavour of the wine. Many ketones are fermentation by-products and only a few seem to have sensory significance [22]. The ketone, 3-octanone, was detected in the tomato wine only after fermentation but not after storage. The (E)-5,9-undecadien-2-one level in the tomato wine, however, experiences significant increase during storage.

Before ageing, 2,3-dihydrobenzofuran, a bioactive phytochemical which is known to possess antiangiogenic properties [42], was identified in the tomato wine. However, after bottle ageing it was not detected. This might be due to its being converted to other compounds.

The sulphur compounds identified in the tomato wine are thiazole, 2-isobutylthiazole, 3-methylisothiazole and 5-methylthiazole. Thiazole and 5-methylthiazole were detected only after fermentation. 2-Isobutylthiazole was detected only in the tomato wine stored at 10^o. One of the major compounds which determine the flavour of tomato is 2-isobutylthiazole [13]. The presence or absence of this compound in the wine may influence its tomato flavour.

Organic acids in wine produce a refreshing taste and modify especially the perception of sweetness and other mouthfeel sensations [22]. In wines fatty acid production is based on the must composition and fermentation conditions [43]. The total concentration of fatty acids detected in the tomato wine after fermentation is 57.37 mg/L (7.73% of all volatiles) (Table 2). After storage at 15^o, even though there is a reduction in the total fatty acid content of the wine, it is not significant (P>0.05). However, there is a significant reduction (P<0.05) after storage at 10^o. This is in contrast with the results of a previous study [35]. The reduction in fatty acids may be due to chemical esterification between alcohols and acids [34]. Octanoic and hexanoic acids are the major acids found in the tomato wine and after storage these two acids show significant reduction. It has been shown that hexanoic and octanoic acids can contribute to the aroma of some white wines [44]. Heptanoic and acetohydroxamic acids were not detected in the wine after fermentation but were formed during storage. The acetic acid content after fermentation is 2.29 mg/L but this increases to 3.23 mg/L after storage at 10^o. These are far below 0.7-1.1 g/L, the level considered objectionable in wines [45]. *S. bayanus*, which was used in this study, is known to produce lower quantities of acetic acid than does *S. cerevisiae* [46]. This may account for the low acetic acid concentration in the tomato wine.

Higher alcohols are secondary products which originate from yeast metabolism during alcoholic fermentation and are important aroma components of wines [8, 22]. They may contribute positively or negatively based on the type and concentration [47]. After fermentation, the total concentration of higher alcohols in the tomato wine is 163.15 mg/L (21.97% of all volatile compounds) (Table 2), and is extremely high compared with the results reported for raspberry wines [48]. After ageing at 10^o and 15^o, it decreases to 103.38 mg/L (13.68% of total volatile compounds) and 110.12 mg/L (14.07% of total volatile compounds) respectively. It is known that the higher alcohol concentration of less than 300 mg/L contributes positively to the aroma of wines but that greater than 400 mg/L may reduce its aroma quality [34]. Therefore the higher alcohol concentrations obtained in this study are likely to contribute positively to the overall aroma of tomato wine. The major higher alcohol detected after fermentation is 3-methyl-1-butanol (isoamyl alcohol), which constitutes 92.77% of all higher alcohols. In a study involving three varietal wines, one of the main alcohols reported is also 3-methyl-1-butanol [15]. After storage the concentration of higher alcohols decreases significantly ($P<0.05$), and the major alcohol, 3-methyl-1-butanol, constitutes 85.61% and 89.73% of all higher alcohols stored at 10^o and 15^o respectively. Storage temperature has a significant effect ($P<0.05$) on the higher alcohol concentration after ageing. The reduction in the concentration after ageing is consistent with the result of a previous study [35] and may be due to chemical esterification [34]. On the other hand, 2-methyl-1-propanol (isobutyl alcohol), 3-ethoxy-1-propanol and 6-octen-1-ol were not detected after fermentation, but only detected after ageing. Reductive denitrification of amino acids or synthesis from sugars [22] might account for this.

Terpenes are secondary products of plants and their biosynthetic pathway starts from acetyl-CoA [49]. It is known that terpenes could play an essential role in the characterisation of wine varieties [15]. In this study only one terpene, 3,7-dimethyl-1,6-octadien-3-ol (linalool), is detected in the tomato wine (Table 2). Linalool was among the terpenes previously reported in three varietal wines [15] and Muscat and Pedro Ximenez wines [21]. The linalool content of the tomato wine stored at 15^o is significantly higher ($P<0.05$) than that stored at 10^o. Linalool is noted for its fruity, rose and citric notes [26].

OAVs and Relative Odour Contribution of Volatile Compounds

The contribution of each volatile compound was assessed by its OAV, the ratio of its concentration to its odour threshold, which was obtained from literature [31, 37, 40, 49, 50]. Those compounds with OAVs greater than 1 are considered to contribute to the wine aroma [31], though it is known that those compounds with OAVs less than 1 can synergistically make a contribution [51]. Compounds in tomato wine with OAVs greater than 1 and their odour descriptors are shown in Table 3. In all, 23 compounds register OAVs greater than 1. Nonanal, decanal, ethyl acetate and octanoic acid, which are among the odour-active compounds found in this study were also identified in a previous study [15]. Vilanova et al. [38] also reported constituents with OAVs greater than 1 in Spanish Albariño wines.

The relative odour contribution (ROC), which indicates the per cent contribution of each volatile compound with OAV greater than 1 is expressed as the ratio of the OAV of the individual compound to the total OAV expressed as percentage [31]. After fermentation the combined ROC of ethyl octanoate, ethyl hexanoate and isoamyl acetate to the aroma of the tomato wine is 98.44%

(Table 3). After ageing the combined ROC values of these three compounds decrease only slightly, i.e. 98.07% and 98.04% for wine stored at 10° and 15 ° respectively. It was reported that the joint contribution of the same three compounds to the aroma of three varietal wines was in the range of 92.9-98.7% [15], which is comparable to the present results. Another study also reported these three constituents as the most contributory compounds to the aroma of Spanish Albariño wines [38]. The odour description of ethyl octanoate is 'sweet, fruity and fresh' [50] while that of ethyl hexanoate is 'apple, fruity and sweetish' [38] and that of isoamyl acetate is 'banana and pear' [31]. Linalool, one of the most odoriferous terpenes with a fruity, rose and citric descriptor [26] gives an ROC value of 0.36%, which increases to 0.38% and 0.48% after storage at 10° and 15° respectively. Linalool thus also contributes much to the global aroma of the tomato wine after storage.

Table 3. Odour activity values (OAVs) and relative odour contribution (ROC) of tomato wine

Compound	C	C10	C15	Odour descriptor
Esters				
Ethyl acetate	1.88 (<0.01%)	2.11 (<0.01%)	2.25(<0.01%)	Fruity, sweet
Ethyl propanoate	ND	18.00 (0.07%)	22.00 (0.08%)	Fruity
Ethyl butanoate	135.50 (0.58%)	149.00 (0.59%)	177.50(0.66%)	Floral, fruity
Ethyl hexanoate	5110.00 (21.85%)	5792.14 (22.99%)	7452.86 (27.67%)	Apple, fruity, sweetish
Ethyl octanoate	17331.50 (74.12%)	18395.00 (73.00%)	18331.50 (68.07%)	Sweet, fruity and fresh
Ethyl nonanoate	ND	3.00 (0.01%)	1.84 (<0.01%)	Cognac, fatty, oily
Ethyl decanoate	20.29 (0.09%)	66.73 (0.27%)	50.26 (0.19%)	Flowery, fruity
Isoamyl acetate	577.33 (2.47%)	525.33 (2.08%)	619.33 (2.30%)	Banana, pear
Diethyl succinate	24.71 (0.11%)	40.29 (0.16%)	31.57 (0.01%)	Light fruity
Methyl octanoate	30.65 (0.13%)	28.30 (0.11%)	30.65 (0.11%)	Intense citrus
Hexyl acetate	0.34 (<0.01%)	0.66 (<0.01%)	0.64 (<0.01%)	Sweet, perfume
2-Phenylethyl acetate	ND	10.00 (0.04%)	ND	Floral, rose, fruity, honey
Higher alcohols				
Isoamyl alcohol	2.52 (0.01%)	1.48 (<0.01%)	1.65 (<0.01%)	Solvent, sweet, nail polish
Isobutyl alcohol	ND	6.51 (0.03%)	-	Malty
3-Ethoxy-1-propanol	ND	6.40 (0.03%)	3.80 (0.01%)	Malty
3-Hexen-1-ol	2.05 (<0.01%)	1.25 (<0.01%)	1.40 (<0.01%)	Green, floral
1-Heptanol	1.70 (<0.01%)	2.19 (<0.01%)	1.77 (<0.01%)	Grape, sweet
1-Octanol	19.33 (0.08%)	15.67 (0.06%)	17.33 (0.06%)	Intense citrus, roses
1-Nonanol	ND	ND	12.07 (0.04%)	
Fatty acids				
Hexanoic acid	4.13 (0.02%)	3.6 (0.01%)	2.9 (0.01%)	Cheese, rancid, fatty, fruity
Octanoic Acid	4.18 (0.02%)	0.44 (<0.01%)	3.68 (0.01%)	Rancid, fatty acid, dairy
Terpene				
Linalool	84.4 (0.36%)	95.60 (0.38%)	129.20 (0.48%)	Fruity, citric
Sulphur compound				
Thiazole	5.26 (0.02%)	ND	ND	Popcorn, peanut

Note: C = tomato wine before ageing; C10 and C15 = tomato wine aged at 10° and 15° respectively. Values in brackets indicate ROC values.

Maejo Int. J. Sci. Technol. **2014**, *8*(02), 129-142

CONCLUSIONS

The volatile profiles of tomato wine before and after storage have been investigated. Ethyl octanoate, ethyl hexanoate and isoamyl acetate, which are characterised by fruity notes, are the main contributors to the tomato wine aroma, both before and after storage. While the concentrations of most odour compounds which have desirable flavour descriptors are observed to increase during storage, those with less desirable flavour characteristics tend to drop.

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